

RECEIVED

1000

2007 FEB 23 AM 7:27

201-16445V

I U C L I D

Data Set

Existing Chemical : ID: 68515-47-9
CAS No. : 68515-47-9
EINECS Name : Di-tridecyl Phthalate
EC No. : 271-089-3
IUPAC Name : 1,2-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich
Molecular Weight : 526

Producer related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 18.10.2000

Substance related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 18.10.2000

Status :
Memo : ACC Phthalate Ester Panel HPV Testing Group

Printing date : 07.12.2006
Revision date :
Date of last update : 07.12.2006

Number of pages : 31

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 68515-47-9
Date 07.12.2006

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : lead organisation
Name : ACC Phthalate Esters Panel HPV Testing Group
Contact person : Dr. Marian Stanley
Date :
Street : 1300 Wilson Blvd.
Town : 22209 Arlington, VA
Country : United States
Phone : (703) 741-5623
Telefax : (703) 741-6091
Telex :
Cedex :
Email :
Homepage :

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes eleven CAS numbers (see the Freertext Remark section for complete list).

Remark : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following eleven CAS numbers:
68648-93-1 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)

117-84-0 1,2,-benzenedicarboxylic acid, dioctyl ester (DOP)

16883-83-3 1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)

68515-40-2 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)

68515-45-7 1,2,-benzenedicarboxylic acid, dinonyl ester, branched and

linear (DNP)

68515-43-5 1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)

84-77-5 1,2-benzenedicarboxylic acid, didecyl ester (DDP)

3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (DUP)

85507-79-5 1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)

111381-91-0 1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)

68515-47-9 1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250°C) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

08.05.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type

:

1. General Information

Id 68515-47-9
Date 07.12.2006

Substance type : organic
Physical status : liquid
Purity :
Colour :
Odour :

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Polymers industry

Remark : High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 68515-47-9

Date 07.12.2006

2.1 MELTING POINT

Value	: -37 °C
Decomposition	: no, at °C
Sublimation	: no
Method	: other: calculated
Year	:
GLP	:
Test substance	: other TS: ditridecyl phthalate ester (CAS No. 68515-47-9)
Remark	: Physicochemical data for 18 commercial phthalate esters from various sources including the public literature, manufacturing specifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data including the values for melting point represent the definitive and currently accepted physicochemical database for selected phthalate esters including ditridecyl phthalate. There were no data on purity. Identified data sources included: Howard P, Banerjee S and Robillard K (1985). Measurement of water solubilities, octanol/water partition coefficients and vapor pressures of commercial phthalate esters. Environ. Tox. Chem 4, 653-661. Howear P (1989). Handbook of Environmental Fate and Exposure Data for Organic Chemicals: Vol I. Large Production and Priority Pollutants. Lewis Publishers, Inc., Chelsea, MI, USA. Sears J and Turchette N (1982). Plasticizers, In: Kirk-Othmer Encyclopedia of Chemical Technology, Eds. Mark H, Othmer D, Overberger C and Seaborg G. Vol. 18, 3rd Edition. John Wiley and Sons, New York, NY, USA.
Test substance	: ditridecyl phthalate ester (CAS No. 68515-47-9)
Reliability	: (2) valid with restrictions Although the original reference was not retrieved and reviewed for quality, this robust summary has a reliability rating of 2 because the data are from a peer reviewed database.
Flag	: Critical study for SIDS endpoint
05.06.2006	(12)
Value	: 177 °C
Decomposition	: no, at °C
Sublimation	: no
Method	: other: calculated
Year	:
GLP	:
Test substance	: other TS: ditridecyl phthalate ester (CAS No. 68515-47-9)
Method	: The calculated value was determined using MPBPWIN version 1.40, a subroutine within the computer program EPIWIN version 3.04. Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula $T_m = 0.5839T_b$, where T_m is the melting point in Kelvin and T_b is the boiling point in Kelvin. The SMILES notation used in the calculation was: <chem>O=C(c1cccc1C(=O)OCCCCCCCCC(C)(C)C)OCCCCCCCCC(C)(C)C</chem>
Remark	: The EPIWIN suite of models is used by the US EPA for estimating chemicophysical properties of substances. However, the melting point

2. Physico-Chemical Data

Id 68515-47-9

Date 07.12.2006

Test substance : calculation in EPIWIN provides erroneously high results for phthalate esters.
Reliability : ditridecyl phthalate ester (CAS No. 68515-47-9)
05.06.2006 : (3) invalid (6)

2.2 BOILING POINT

Value : 501 °C at 1013 hPa
Decomposition : no
Method : other: calculated
Year :
GLP :
Test substance : other TS: ditridecyl phthalate ester (CAS No. 68515-47-9)
Method : Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark : EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance : ditridecyl phthalate ester (CAS No. 68515-47-9)
Reliability : (2) valid with restrictions
07.12.2006 (6)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .000000000363 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: ditridecyl phthalate ester (CAS No. 68515-47-9)
Remark : Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, handbook values, and computer modeling were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for vapour pressure represent the definitive and currently accepted physicochemical database for selected phthalate esters including ditridecyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm³ mol⁻¹). The Le Bas molar volume used for ditridecyl phthalate ester was 742.4 cm³ mol⁻¹.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r² = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)

2. Physico-Chemical Data

Id 68515-47-9

Date 07.12.2006

 $r^2 = 0.87$, SE = 0.33Log CS(OL) = $-0.016V + 3.4$, n = 68 (solubility in octanol) $r^2 = 0.19$, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance**Reliability**

: ditridecyl phthalate ester (CAS No. 68515-47-9)

: (2) valid with restrictions

The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag

05.06.2006

: Critical study for SIDS endpoint

(4)

Value

: .00000000093 hPa at 25 °C

Decomposition

: no

Method

: other (calculated)

Year

:

GLP

:

Test substance

: other TS: ditridecyl phthalate ester (CAS No. 68515-47-9)

Method

: Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04.

Vapor Pressure estimations performed by MPBPWIN are based on the calculation method of Grain, which uses boiling point for the calculation. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985. The SMILES notation used in the calculation was:

O=C(c1cccc1C(=O)O)OCCCCCCCC(C)(C)OCCCCCCCC(C)(C)C**Remark**

: The EPIWIN suite of models is used by the US EPA for estimating chemico-physical properties of substances.

Test substance

: ditridecyl phthalate ester (CAS No. 68515-47-9)

Reliability

: (2) valid with restrictions

The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

05.06.2006

(6)

2.5 PARTITION COEFFICIENT

Partition coefficient

: octanol-water

Log pow

: = 12.06 at 25 °C

pH value

:

Method

: other (calculated)

Year

:

GLP

:

Test substance

: other TS: ditridecyl phthalate ester (CAS No. 68515-47-9)

Remark

: Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, handbook values, and computer modeling were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for octanol-water partitioning represent the definitive and currently accepted physicochemical database for selected phthalate esters including ditridecyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level,

2. Physico-Chemical Data

Id 68515-47-9

Date 07.12.2006

were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm³ mol⁻¹). The Le Bas molar volume used for dodecyl phthalate ester was 742.4 cm³ mol⁻¹.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r² = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r² = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r² = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : dodecyl phthalate ester (CAS No. 68515-47-9)
Reliability : (2) valid with restrictions

The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
06.07.2006

(4)

Partition coefficient : octanol-water
Log pow : 12.25 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance : other TS: dodecyl phthalate ester (CAS No. 68515-47-9)

Method : The value was calculated using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Octanol / Water Partition Coefficient estimations performed by KOWWIN are based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. J. Pharm. Sci. 84:83-92.

The SMILES notation used in the calculation was:

Remark : O=C(c1cccc1C(=O)OCCCCCCCCC(C)(C)C)OCCCCCCCCC(C)(C)C
The EPIWIN suite of models is used by the US EPA for estimating chemico-physical properties of substances.

Test substance : dodecyl phthalate ester (CAS No. 68515-47-9)
Reliability : (2) valid with restrictions

The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

05.06.2006

(6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : = .00007 other: ug/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :

2. Physico-Chemical Data

Id 68515-47-9

Date 07.12.2006

Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: ditiidecyl phthalate ester (CAS No. 68515-47-9)
Remark	:	<p>Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, handbook values, and computer modeling were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for water solubility represent the definitive and currently accepted physicochemical database for selected phthalate esters including ditiidecyl phthalate.</p> <p>Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm³ mol⁻¹). The Le Bas molar volume used for ditiidecyl phthalate ester was 742.4 cm³ mol⁻¹.</p> <p>Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r² = 0.98, SE = 0.39</p> <p>Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r² = 0.87, SE = 0.33</p> <p>Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r² = 0.919, SE = 0.41</p> <p>It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.</p>
Test substance	:	ditiidecyl phthalate ester (CAS No. 68515-47-9)
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
05.06.2006		(4)
Solubility in	:	Water
Value	:	= .00002 other: ug/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: ditiidecyl phthalate ester (CAS No. 68515-47-9)
Method	:	Water solubility calculated by WSKOWWIN, a subroutine of the computer program EPIWIN version 3.04. that is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". Environ. Toxicol. Chem. 15:100-106. 1995.

2. Physico-Chemical Data

Id 68515-47-9

Date 07.12.2006

Remark

The SMILES notation used in the calculation was:
O=C(c1cccc1C(=O)OCCCCCCCCC(C)(C)C)OCCCCCCCCC(C)(C)C

Test substance

: The EPIWIN suite of models is used by the US EPA for estimating chemicophysical properties of substances.

Reliability

: ditridecyl phthalate ester (CAS No. 68515-47-9)

: (2) valid with restrictions

The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

05.06.2006

(6)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 68515-47-9

Date 07.12.2006

3.1.1 PHOTODEGRADATION

Type : air
Light source : Sun light
Light spectrum : nm
Relative intensity : 1 based on intensity of sunlight
Conc. of substance : at 25 °C
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : = .000000000246 cm³/(molecule*sec)
Degradation : = 50 % after 5 hour(s)
Deg. product :
Method : other (calculated)
Year :
GLP :
Test substance : other TS: ditridecyl phthalate ester (CAS No. 68515-47-9)

Method : Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04.
Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson.
Remark : 50% degradation after 5.0 hrs or 0.42 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration.
EPI SuiteTM is used by the US EPA for estimating chemicophysical properties of substances.
Test substance : ditridecyl phthalate ester (CAS No. 68515-47-9)
Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
06.07.2006 (6)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : = 7.7 year at 25 °C
t1/2 pH9 : at °C
Deg. product : not measured
Method : other (calculated)
Year :
GLP :
Test substance : other TS: ditridecyl phthalate ester (CAS No. 68515-47-9)

Method : Hydrolysis rate calculated by HYDROWIN ver. 1.67, a subroutine of the computer program EPIWIN version 3.04, that is based on work for EPA by T. Mill et al.
Remark : The EPIWIN suite of models is used by the US EPA for estimating chemicophysical properties of substances.
Test substance : ditridecyl phthalate ester (CAS No. 68515-47-9)

3. Environmental Fate and Pathways

Id 68515-47-9

Date 07.12.2006

Reliability : (2) valid with restrictions
The value was calculated based on chemical structure as modeled by EPIWIN. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
06.07.2006 (6)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1997

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model were:

MW = 530.8

Temperature = 25C

Water Solubility = 0.00000007 mg/L

Vapor Pressure = 3.63E-8 Pa

Pow = 12.1

Melting Point = -37C

Result : Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Soil = 97.7%
Air = 0.0%
Water = 0.0%
Sediment = 2.2%
Suspended sed. = 0.1%
Biota = 0.0%

Test substance : ditridecyl phthalate ester (CAS No. 68515-47-9)
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
05.06.2006 (9)

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

3. Environmental Fate and Pathways

Id 68515-47-9

Date 07.12.2006

Remark

: Physicochemical input values for the model to represent a dinitridecyl phthalate ester were:

MW = 530.8

Temperature = 25C

Water Solubility = 0.00000007 mg/L

Vapor Pressure = 3.63E-8 Pa

Pow = 12.1

Melting Point = -37C

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
-------------	--------------

Air	0 (based on negligible VP)
-----	----------------------------

Water	0 (based on negligible WS)
-------	----------------------------

Soil	300 (compartment emitted to based on Pow)
------	---

Half-lives used in the calculation:

Compartment	Half-life (hr)
-------------	----------------

Air	5.0a
-----	------

Water	2400b
-------	-------

Soil	8400c
------	-------

Sediment	8400c
----------	-------

a - as calculated using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04 [Environmental Protection Agency (EPA) (2000). EPI Suite™, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from Staples et al. (1997), Sugatt et al. (1983) and Boethling (2000):

Staples C, Peterson D, Parkerton T and Adams W (1997). The environmental fate of phthalate esters: A literature review. Chemosphere 35, 667-749.

Sugatt R, O'Grady D, Banerjee S and Howard P (1983). Shake flask biodegradation of 14 commercial phthalate esters. SRC# L1543-05. Final report submitted to Chemical Manufacturers Association, Washington, D.C., USA.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment).

Result

: Using the Mackay Level III calculation, the following distribution is predicted for dinitridecyl phthalate ester:

Compartment	%Distribution
-------------	---------------

Air	<0.01
-----	-------

3. Environmental Fate and Pathways

Id 68515-47-9

Date 07.12.2006

Water <0.01
Soil 99.92
Sediment 0.07
Test substance : ditridecyl phthalate ester (CAS No. 68515-47-9)
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

05.06.2006

(8)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted
Concentration : 52 mg/l related to Test substance
related to
Contact time : 56 day(s)
Degradation : = 62.7 (±) % after 56 day(s)
Result :
Kinetic of testsubst. : 28 day(s) = 12.8 %
%
%
%
%
Deg. product :
Method : OECD Guide-line 301 F "Ready Biodegradability: Manometric
Respirometry Test"
Year :
GLP : no
Test substance : other TS: 1,2-benzenedicarboxylic acid, diiso-C13 alkyl esters (CAS No. 68515-47-9)
Result : The biodegradation half-life <7 weeks. By days 28 and 56, 12.8 and 62.7% degradation, respectively, of the test substance was observed. 10% biodegradation was achieved on approximately day 27 and 50% biodegradation on approximately day 47.

By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. Oxygen uptake of the blanks were within guideline limits. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test substance as calculated using results of an elemental analysis of the test substance.

Test Substance:

Day	% Degradation*
7	0, 0, 0
14	0, 0, 1
21	1, 5, 1
28	1, 26, 11 (mean = 12.8)
56	59, 68, 62 (mean = 62.7)

Positive Reference Substance (Na Benzoate):

Day	% Degradation*
4	82, 80
5	87, 85

3. Environmental Fate and Pathways

Id 68515-47-9

Date 07.12.2006

Test condition	<p>* replicate data</p> <p>: Activated sludge and test medium were combined prior to test substance addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, calcium chloride).</p> <p>Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test substance was tested in triplicate, controls and blanks were tested in duplicate.</p> <p>Test substance (1,2-benzenedicarboxylic acid, diiso-C13 alkyl esters) concentration was approximately 52 mg/L. The positive control (sodium benzoate) concentration was approximately 50 mg/L. Test temperature was 22 +/- 1 Deg C.</p> <p>All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.</p>
Test substance	: 1,2-benzenedicarboxylic acid, diiso-C13 alkyl esters (CAS No. 68515-47-9) No information on purity, but believed to be 100% commercial product.
Conclusion	: The test substance is not readily biodegradable.
Reliability	: (1) valid without restriction This summary is rated a "1" and represents a key study because it followed an OECD standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.
Flag 05.06.2006	: Critical study for SIDS endpoint (7)
Type	: aerobic
Inoculum	: domestic sewage
Concentration	: 20 mg/l related to Test substance related to
Contact time	: 28 day(s)
Degradation	: = 37 (±) % after 28 day(s)
Result	: other
Deg. product	:
Method	: other
Year	:
GLP	: no data
Test substance	: other TS: ditridecyl phthalate ester (CAS No. 68515-47-9)
Method	: Method/Guideline - USEPA 1982, CO2 Evolution, Shake Flask (modified Gledhill). Inoculum - Domestic sewage, soil, and mineral medium. Kinetics - Not Reported Degradation Products - Not Reported Analytical Monitoring - Yes
Result	: Primary degradation is expressed as the loss of initial test substance. Ultimate biodegradation is expressed as the percentage of ThCO2 in each flask.
Test condition	: >50% primary biodegradation occurred and 37.0% (sd 10) ultimate biodegradation. The test substance was continuing to degrade at 28 days. Inoculum was aged for 2 weeks prior to test initiation. The test chemical was added to flasks containing medium and inoculum. The flasks were incubated and shaken in the dark for 28 days. Three replicates for CO2 evaluation and 4 replicates for primary degradation were tested. The CO2 production was captured in barium hydroxide solution. Primary biodegradation was determined at the beginning, middle and end by GC FID of entire contents of one replicate. A glucose and blank were also tested..

3. Environmental Fate and Pathways

Id 68515-47-9
Date 07.12.2006

2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120rpm at 22 +/- 2 Deg C.

Test substance : Nominal test concentration = 20mg/L for test substance and glucose.
Ditridecyl Phthalate (CAS# 68515-47-9)
(1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters C13 rich)
Synonym: DTDP
No information on purity, but DMP was analytically confirmed to be within commercial specifications.

Reliability : (2) valid with restrictions
06.07.2006 (12) (14)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

Id 68515-47-9

Date 07.12.2006

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : flow through
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : > .15
Limit test :
Analytical monitoring : yes
Method : other
Year : 1975
GLP : yes
Test substance : other TS: Ditridecyl Phthalate Ester (CAS# 68515-47-9)

Method : Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians.

Remark : Statistical methods-Moving average angle, Probit or Bionomial concentration.
: Control mortality occurred in the study. The mortality occurred in one of the two control replicate systems. The mortality was considered to have been caused by contamination in the one test system. Because no mortality occurred in any treatments and the second control system, the results were assessed as valid.

Result : 96 hr LC50 >0.15 mg/L
Mean measured values were used in the LC50 calculation.

Nominal test concentrations: control, 0.018, 0.036, 0.072, 0.14, and 0.29 ul/L.
Mean measured test concentrations: <0.0094, 0.013, 0.023, 0.039, 0.067, and 0.15 mg/L.

Analytical samples were taken at time zero and on a composite of replicates at study termination. Measured values dropped slightly during the exposure period.

% Mortality results at 96 hrs per replicate for control and treatment levels:
Conc. (mg/L) Rep1/Rep2

Control	0 / 10
0.013	0 / 0
0.023	0 / 0
0.039	0 / 0
0.067	0 / 0
0.15	0 / 0

Test condition : Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15 L of solution. The diluter maintained a water turnover rate of 5 to 8 tank volumes per day. Two replicates of ten organisms were tested per treatment and control. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection.

Fish mean length = 39 mm and mean wet weight = 0.5 g. Test temperature = 11 Deg C. The pH ranged from 7.1 to 7.5. The mean dissolved oxygen ranged from 9.8 to 10.0 mg/L. Ranges of total hardness

4. Ecotoxicity

Id 68515-47-9

Date 07.12.2006

and alkalinity as CaCO₃ of the dilution water were 20 to 26 mg/L and 14 to 22 mg/L, respectively.

Test substance : Fish were obtained from a Montana supplier.
Ditridecyl Phthalate (CAS# 68515-47-9)
(1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters C13 rich)
Synonym: DTDP
Purity: 100% active ingredient

Conclusion : Test substance is non-toxic to fish at or below its water solubility level.
Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability : (1) valid without restriction
This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

Flag : Critical study for SIDS endpoint
05.06.2006 (5) (13)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : > .05 measured/nominal
Analytical monitoring : yes
Method : other
Year : 1975
GLP : yes
Test substance : other TS: Diisotridecyl Phthalate Ester (CAS No. 68515-47-9)

Method : Method/Guideline - U.S. EPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975.
Statistical methods incorporated the following procedures: Moving average angle, Probit, and Binomial Probability.

Result : 48 hr EC50 >0.068 mg/L (based upon time zero analytical samples; no effects at test substance saturation). Value was recalculated as >0.05 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).

Mean measured values were used in the final EC50 calculation.

Nominal test concentrations: control, 0.032, 0.055, 0.090, 0.15, and 0.25 ul/L.

Mean measured test concentrations of time 0 and 48 hr values: <0.0088, <0.0088, 0.011, 0.017, 0.029, and 0.055 mg/L.

Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined to a level at or below the detection limit during study exposure. The high treatment solution is considered the maximum solubility achievable under the conditions of the test.

% Immobility results at 48 hrs per replicate for control and treatment levels:
Conc. (mg/L) Rep1/Rep2/Rep3

Control	0 / 0 / 0
<0.0088	0 / 0 / 0
0.011	0 / 0 / 0

4. Ecotoxicity

Id 68515-47-9

Date 07.12.2006

	0.017	0 / 0 / 0
	0.029	0 / 0 / 20
	0.055	0 / 0 / 0
Test condition	:	Test treatments for the initial test were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 30 minutes. The stock solution was prepared at the highest treatment concentration. Dilutions of the stock were prepared for each treatment level. Three replicates of five organisms were tested per treatment. Test vessels were 250 ml beakers with 200 ml of test solution. Analytical method was Gas Liquid Chromatography (GLC).
Test substance	:	Test temperature = 22 Deg C. The pH was 8.3 at initiation and 8.4 on day 2. Dissolved oxygen ranged from 8.7 to 9.1 at initiation and 7.6 to 7.9 on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock. Ditridecyl Phthalate Ester (DTDP, CAS# 68515-47-9) (1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters C13 rich) Synonym: DTDP Purity: unstated, but believed to be 100% active ingredient because the test material came from the same source as in the rainbow trout acute study.
Conclusion	:	Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).
Reliability	:	(1) valid without restriction This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.
Flag	:	Critical study for SIDS endpoint
07.12.2006		(10) (13)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Selenastrum capricornutum (Algae)
Endpoint	:	other: biomass and growth rate
Exposure period	:	8 day(s)
Unit	:	mg/l
NOEC	:	= .6
EC50	:	> .6 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	1978
GLP	:	yes
Test substance	:	other TS: Ditridecyl Phthalate Ester (DTDP, CAS# 68515-47-9)
Method	:	Method/Guideline - U.S. EPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978. Statistical methods - Moving average angle, Probit or Bionomial Test type - Static
Result	:	192 hr (8 day) EC50 >1.0 mg/L (based upon time zero analytical samples). Value was recalculated as >0.6 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997). Mean measured values were used in the final EC50 calculation. Nominal test concentration as a percent of a saturated solution: 0 (control)

and 100.0%.

Mean measured test concentrations of time 0 and 144 hr values: <0.10 and 0.6 mg/L (detection limit was 0.10 mg/L).

Analytical samples taken at time zero and on a composite of replicates at termination. In-vivo chlorophyll a, measured until less than 5% change. Both cell number and in-vivo chlorophyll a, measured at termination. Control chlorophyll a or cell counts were not reported. A stimulatory effect of 21 and 23% as compared with the control for chlorophyll a was measured on days 6 and 8, respectively. Analytical samples were taken at time zero and on a composite of replicates at termination.

Chlorophyll a percent change relative to control on sampling days and cell number on day 8 results:

Conc. Chlorophyll a percent change from control
(mg/L) Day 1 Day 2 Day 4 Day 6 Day 8 Cell # Day 8
0.6 -26 -1 -10 +21 +23 +14

Test condition

: Algal Growth Medium was used as the control and diluent. 10 uL of test substance was added to 1.0 L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0 E4 cells/ml. Only one treatment level was evaluated (100% WSF) because earlier phthalate testing suggested that toxic effects were not expected with higher molecular weight phthalate esters with low water solubility.

Test substance

Lighting = 4,700 lux, Test temperature = 22+/-2 Deg C. The pH was 7.4 at initiation and ranged from 8.4 to 8.6 on day 8. Algal culture stock was obtained from University of Texas at Austin, TX.
: Ditridecyl Phthalate Ester (CAS# 68515-47-9)
(1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters C13 rich)
Synonym: DTDP
Purity: unstated, but believed to be 100% active ingredient as was provided in the rainbow trout study.

Conclusion

: Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al (1997).

Reliability

: (1) valid without restriction
The study procedure followed an accepted test guideline and applied GLP. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances. Control chlorophyll or cell counts not reported.

Flag

07.12.2006

: Critical study for SIDS endpoint

(11) (13)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA**4.5.1 CHRONIC TOXICITY TO FISH****4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES**

Species : Daphnia magna (Crustacea)
Endpoint : reproduction rate
Exposure period : 21 day(s)
Unit : mg/l
NOEC : = .9

4. Ecotoxicity

Id 68515-47-9

Date 07.12.2006

EC50 : > .9
Analytical monitoring : yes
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year : 1984
GLP : yes
Test substance : other TS: Diisotridecyl Phthalate Ester (CAS No. 68515-47-9)

Method : The test method followed the Daphnid chronic testing procedure described in OECD guideline 202 (1984) with the use of a dispersant, castor oil 40-ethoxylate (Marlowet 40), in accordance with guideline specifications.

Result : Daphnia parent (Po) survival, reproduction (cumulative number of offspring, F1, per live parent), and parent length were evaluated as the biological endpoints. Diisotridecyl phthalate ester showed no effect on survival, reproduction, and length at a loading of 1.0 mg/L test substance and 10 mg/L dispersant under the conditions of this test.

	Po % Mortality	Mean F1/Surviving Po	Po Po Mean Length
Test Substance	0	138 (sd=12.3)	4.4 (sd=0.17)
Control	0	120 (sd=13.3)	4.2 (sd=0.14)

	Control	Dispersant Control	Test Substance
Po % Mortality	0	20	0
Mean F1/			

Surviving Po	120 (sd=13.3)	131 (sd=23.5)	138 (sd=12.3)
--------------	---------------	---------------	---------------

Po Mean Length	4.2 (sd=0.14)	4.3 (sd=0.16)	4.4 (sd=0.17)
----------------	---------------	---------------	---------------

Test condition : Test substance exposure solutions were prepared using stock dispersions prepared by adding 100 mg substance and 1000 mg dispersant (castor oil 40-ethoxylate; Marlowet 40), then bringing the test solution to 1 L by adding dilution medium. The dilution medium was Elendt's medium (Elendt and Bias, 1990), which was pH adjusted to 8 and aerated for >2 hours prior to use.

Ten replicate test systems with 1 daphnid each (< 24 hours old) were prepared in glass beakers with loose fitting lids. Each beaker contained 80 ml of exposure solution with a depth of approximately 5 cm. The photoperiod was controlled to 16 hours light and 8 hours dark with a 15 minute transition period.

The exposure solution was renewed every Monday, Wednesday, and Friday. On each renewal day the parent organism (Po) was transferred to a new exposure solution and neonates (F1) were counted. Water quality measurements including dissolved oxygen concentration and pH were determined at every renewal for the new and old exposure and control solutions. Test conditions were:

Temperature = 20 +/- 1.0 degree C

Water hardness = >140 mg/L (as CaCO3)

Alkalinity = >100 mg/L (as CaCO3)

pH = approximately 8

Dissolved oxygen = 8-9 mg/L

Standard daily feeding rates with the cultured alga, *Chlorella vulgaris*, was supplemented with microencapsulated food, "Frippak Booster". This rate was increased by 10% from day 5 of the test as data from earlier studies indicated that additional feed was appropriate to prevent stress due to food deficiency.

Test substance analyses of new and old exposure solutions were performed using gas chromatography with flame ionization detection, after a hexane extraction. The mean measured test substance concentrations were 0.91 mg/L in new exposure solutions and 0.90 mg/L in old exposure solutions, which represents 91 and 90%, respectively, of the nominally added test substance.

4. Ecotoxicity

Id 68515-47-9

Date 07.12.2006

Test substance	: Diisotridecyl Phthalate Ester (CAS No. 68515-47-9); purity >99.5%
Conclusion	: Chronic invertebrate (<i>Daphnia magna</i>) toxicity data reported for diisotridecyl phthalate ester are consistent with valid data for several high molecular weight phthalate esters as summarized by Brown et al. (1998), Staples et al. (1997), and Rhodes et al. (1995). These data show that high molecular weight phthalate esters, including diisotridecyl phthalate ester, do not produce chronic toxicity to <i>Daphnia magna</i> . Testing was conducted at a loading that exceeds the water solubility of diisotridecyl phthalate ester (expected to be less than 0.17 ug/L, which was determined for a diisodecyl phthalate ester; Letinski et al., 2002) after it was demonstrated that such a procedure was able to satisfactorily disperse the test substance and that it prevented floatation of the test organism, a documented problem that can occur when evaluating the toxicity of similar substances.
Reliability	: (1) valid without restriction The study procedure followed an accepted test guideline and applied GLP. The study procedure and results were accepted in a peer reviewed journal. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.
Flag	: Critical study for SIDS endpoint
05.06.2006	(3)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : > 10000 mg/kg bw
Species : rat
Strain : Sprague-Dawley
Sex : male
Number of animals : 35
Vehicle : no data
Doses :
Method : other
Year : 1981
GLP : yes
Test substance : other TS: Diisotridecyl Phthalate Ester (CAS No. 68515-47-9)

Remark : No rats died during the study. The animals were generally free of abnormalities throughout the observation period. There were no significant findings at the terminal sacrifice.

Test condition : Following a 18 hour fasting period, animals were administered the test compound at doses of 1.0, 1.47, 2.15, 3.16, 4.64, 6.81, and 10.0 mg/kg of body weight. Observations were recorded immediately after dosing, then at 1, 2, and 4 hours; and once daily thereafter for 14 days. Body weights were recorded prior to dosing and at 7 and 14 days. Gross necropsies were conducted on all animals that were sacrificed at the termination of the study.

Test substance : Diisotridecyl Phthalate Ester (CAS No. 68515-47-9)
Conclusion : Under the conditions of this study, the test material has a low order of acute oral toxicity.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

07.12.2006 (2)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : > - 3160 mg/kg bw
Species : rabbit
Strain : New Zealand white
Sex : male/female
Number of animals : 8
Vehicle : no data
Doses :
Method : other
Year : 1981
GLP : yes
Test substance : other TS: Diisotridecyl Phthalate Ester (CAS No. 68515-47-9)

Remark : No rabbits died during the study. The animals in the highest dose group (3.16 g/kg) showed weight losses over the first week but all animals gained weight during the second week. Signs of skin irritation were observed

5. Toxicity

Id 68515-47-9

Date 07.12.2006

Test condition	<p>during the first week, ranging from barely perceptible erythema in the lowest doses to moderate/severe erythema in the high dose group. No irritation was observed by the end of the study. There were no significant findings at the terminal sacrifice.</p> <p>: The dose levels were 50, 200, 794, and 3160 mg/kg body weight. On the day prior to dosing the fur of each rabbit was clipped. The skin was intact and not abraded. The test material was applied directly to the skin and evenly spread; the area was wrapped with gauze and an impervious plastic sleeve. The wraps were removed after 24 hours and dermal observations recorded. General observations were recorded immediately after dosing, then at 1, 2, and 4 hours; and once daily thereafter for 14 days. Observations for skin irritation were recorded 30 minutes after removal of the wrap and at Days 3, 7, 10, and 14. Body weights were recorded prior to dosing and at 7 and 14 days. Gross necropsies were conducted on all animals that were sacrificed at the termination of the study.</p>
Test substance	: 1,2-benzenetricarboxylic acid, di-C11-14-branched alkyl esters, C13 rich. (ditridecyl phthalate Ester, DTDPE)
Conclusion	: Under the conditions of this study, the test material has a low order of acute dermal toxicity.
Reliability	: (1) valid without restriction
Flag	: Critical study for SIDS endpoint
07.12.2006	(1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	: Ames test
System of testing	: Bacterial
Test concentration	: 5 dose levels up to 10 mg/plate
Cytotoxic concentr.	:
Metabolic activation	: with and without
Result	: negative
Method	: OECD Guide-line 471
Year	: 1985
GLP	: no data
Test substance	: other TS: Diisotridecyl Phthalate Ester (CAS No. 68515-47-9)
Method	: A mutagenic response was defined as a reproducible, dose-related increase in the number of histidine-independent colonies over the spontaneous incidence. There was no requirement for a specific magnitude of increase.
Test condition	: Approximately 10E8 bacteria were mixed with 0.5 ml of either 0.1M sodium

5. Toxicity

Id 68515-47-9

Date 07.12.2006

phosphate buffer or S-9 mix, and test substance. The reaction was carried out in triplicate. The mixture was incubated at 37°C for 48 hours, after which time histidine-revertant colonies were counted. The doses selected were separated by half-log intervals. The high dose was 10 mg/plate unless limited by solubility. Positive control chemicals were sodium azide, nitro-o-phenylenediamine, 9-aminoacridine and 2-aminoanthracene. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest with TA100 was conducted to determine the high dose level.

Test substance : 1,2-benzenetricarboxylic acid, di-C13-branched alkyl esters (ditridecyl phthalate Ester, DTDP)
Conclusion : No mutagenic activity was observed at doses up to 10 mg/plate in Salmonella strains TA98, TA100, TA1535 and TA1537 with or without metabolic activation.
Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

07.12.2006

(15)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 68515-47-9

Date 07.12.2006

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

- (1) Bio/dynamics, Inc. (1981). Acute Dermal Toxicity in Rabbits. Conducted for Exxon Biomedical Sciences, Inc. Unpublished report.
- (2) Bio/dynamics, Inc. (1981). Acute Oral Toxicity in Rats. Conducted for Exxon Biomedical Sciences, Inc. Unpublished report.
- (3) Brown D, Croudace C, Williams N, Shearing J and Johnson P (1998). The effect of phthalate ester plasticisers tested as surfactant stabilised dispersions on the reproduction of the *Daphnia magna*. *Chemosphere* 36, 1367-1379.
- (4) Cousins I and Mackay D (2000). Correlating the physical-chemical properties of phthalate esters using the 'three solubility' approach. *Chemosphere* 41, 1389-1399.
- (5) EG&G Bionomics, Inc. (1983). Acute Toxicity of Fourteen Esters to Rainbow Trout *Salmo gairdneri* Under Flow-Through Conditions. Report No. BW-83-3-1373. Unpublished report.
- (6) Environmental Protection Agency (EPA) (2000). EPI Suite™, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
- (7) Exxon Biomedical Sciences, Inc. (1999). Ready Biodegradability, Manometric Respirometry. Study No. 169094A. Unpublished report.
- (8) Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.
- (9) Mackay D, DiGuardo A, Paterson S and Cowan C (1997). EQC Model ver. 1.01, available from the Environmental Centre, Trent University, Canada.
- (10) Springborn Bionomics, Inc. (1984). Acute Toxicity of Fourteen Esters to *Daphnia magna*. Report No. BW-84-4-1567. Unpublished report.
- (11) Springborn Bionomics, Inc. (1984). Acute Toxicity of Fourteen Esters to the Freshwater Green Alga *Selenastrum capricornutum*. Report No. BP-84-1-4. Unpublished report.
- (12) Staples C, Peterson D, Parkerton T and Adams W (1997). The environmental fate of phthalate esters: A literature review. *Chemosphere* 35, 667-749.
- (13) Staples CA, et al (1997). Aquatic toxicity of eighteen phthalate esters. *Environmental Toxicology and Chemistry* 16(5), 875-891.
- (14) Sugatt R, O'Grady D, Banerjee S and Howard P (1983). Shake flask biodegradation of 14 commercial phthalate esters. SRC # L1543-05. Final report submitted to Chemical Manufacturers Association, Washington, D.C., USA.
- (15) Zeiger E, Haworth S, Mortelmans K and Speck W (1985). Mutagenicity testing of Di(2-ethylhexyl) phthalate and related chemicals in *Salmonella*. *Environmental Mutagenesis* 7, 213-232.

10.1 END POINT SUMMARY**10.2 HAZARD SUMMARY**

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physicochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

06.07.2006

10.3 RISK ASSESSMENT